Table S2. Comparison of simulated plasma AUC and C_{max} values to those observed clinically.

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
Amodiaquine								
600 mg QD (Day 3)[a]	24.6	28.4	1.16	0 – 24	204	251	1.23	Scarsi et al., 2014 [1]
540 mg SD[f]	41.2	47.6	1.16	0 – 48	331	521	1.57	Liu et al., 2014 [2]
600 mg SD[a]	58.0	23.5	0.40	0 – 48	748	227	0.30	Soyinka et al., 2010 [3]
600 mg SD[e]	24.9	22.9	0.92	0 – 24	234	194	0.83	Akande et al., 2015 [4]
	Within 1.5-fold		**75%**		**Within 1.5-fold**		**50%**	
	Within 2-fold		**75%**		**Within 2-fold**		**75%**	
Artemether								
80 mg SD[a,c]	104	80.5	0.77	0 – inf	320	333	1.04	Lefevre et al., 2002 [5]
80 mg SD[a,k]	113	74.7	0.66	0 – inf	408	327	0.80	Lefevre et al., 2013 [6]
80 mg BID (Day 3 PM)[a,c]	30.8	38.5	1.25	62 – 72	61.4	124	2.02	Lefevre et al., 2002 [7]
80 mg BID (Day 3 PM)[a,c]	21.2	35.0	1.65	60 – 72	59.5	150	2.53	Huang et al., 2012 [8]
	Within 1.5-fold		**75%**		**Within 1.5-fold**		**50%**	
	Within 2-fold		**100%**		**Within 2-fold**		**50%**	
Atovaquone								
500 mg SD[a,c]	4.4[#]	3.8[#]	0.9	Unknown	288[#]	214[#]	0.7	Rolan et al., 1994 [9]
250 mg SD[a,c]	3.7[*]	4.5[*]	1.2	0 – inf	295[*]	295[*]	1.0	Thapar et al., 2002 [10]
250 mg QD[a,c]	13.8[*]	13.9[*]	1.0	0 – 24	254[*]	260[*]	1.0	Thapar et al., 2002 [10]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Azithromycin								
500 mg SD[a]	410	394	0.96	0 – 12	1770	2235	1.26	Foulds et al., 1990 [11]
500 mg BID Day 1 then 500 mg QD (Day 6)[a]	620	500	0.81	0 – 12	3180	3381	1.06	Foulds et al., 1990 [11]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
Carboxyprimaquine								
15 mg SD[a]	NA	NA	NA	0 – 24	15100	14900	0.99	Mihaly et al., 1985 [12]
45 mg SD[a]	NA	NA	NA	0 – 24	39900	44800	1.12	Mihaly et al., 1985 [12]
30 mg SD[g]	959	1700	1.78	0 – inf	44000	53600	1.22	Hanboonkunupakarn et al., 2014 [13]
15 mg SD[g]	736	886	1.20	0 – inf	14200	15900	1.12	Ward et al., 1985 [14]
15 mg QD (Day 14)[g]	1240	1310	1.06	0 – inf	24700	25500	1.03	Ward et al., 1985 [14]
30 mg SD[f]	1040	1740	1.67	0 – inf	47200	50900	1.08	Jittamala et al., 2015 [15]
	Within 1.5-fold		**50%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Chloroquine								
300 mg infusion[a,c] (over 23.5 mins) SD[a,c]	837	881	1.05	0 – inf	7511	8003	1.07	Gustafsson et al., 1983 [16]
300 mg tablet SD[a,c]	76.0	77.9	1.02	0 – inf	6111	7210	1.18	Gustafsson et al., 1983 [16]
300 mg soln. SD[a,c]	73.0	77.9	1.07	0 – inf	4990	7210	1.44	Gustafsson et al., 1983 [16]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Cycloguanil								
200 mg SD[a]	41	73	1.78	0 – inf	661	1080	1.63	Wattanagoon et al., 1987 [17]
200 mg SD EM[a]	NA	NA	NA	0 – inf	3396	1938	0.57	Helsby et al., 1990 [18]
200 mg SD PM[a]	NA	NA	NA	0 – inf	6563	3781	0.58	Helsby et al., 1990 [18]
200 mg SD EM[a]	NA	NA	NA	0 – 72	2350	2560	1.09	Helsby et al., 1993 [19]
200 mg QD (Day 14) EM[a]	NA	NA	NA	0 – 24	3170	2600	0.82	Helsby et al., 1993 [19]
200 mg SD PM[a]	NA	NA	NA	0 – 72	983	229	0.23	Helsby et al., 1993 [19]
200 mg QD (Day 14) PM[a]	NA	NA	NA	0 – 24	1190	314	0.26	Helsby et al., 1993 [19]
	Within 1.5-fold		**0%**		**Within 1.5-fold**		**29%**	
	Within 2-fold		**100%**		**Within 2-fold**		**71%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
DEAQ								
600 mg QD (Day 3)[a]	495	343.26	0.69	0 – 96	14571	17358	1.19	Scarsi et al., 2014 [1]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
DHA								
4 mg/kg SD[f]	360	270	0.81	0 – inf	907	895	0.99	Na-Bangchang et al., 2004 [20]
300 mg SD[f]	646	428	0.63	0 – inf	2018	1316	0.68	Na-Bangchang et al., 1997 [21]
240 mg SD[g]	481	354	0.74	0 – inf	1980	1088	0.55	Le et al., 1999 [22]
120 mg SD[g]	159	145	0.91	0 – inf	370	488	1.32	Chinh et al., 2009 [23]
	Within 1.5-fold		**75%**		**Within 1.5-fold**		**75%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
DHA (administered as artesunate)								
180 mg SD[f]	523	525	1.00	0 – inf	1400	754	0.54	Jittamala et al., 2015 [15]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**0%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Doxycycline								
100 mg SD[a]	1.75[#]	1.60[#]	0.914	0 – inf	29.9[#]	30.3[#]	1.01	Grahnen et al., 1994 [24]
100 mg SD[a]	NA	NA	NA	0 – inf	40.1[#]	30.8[#]	0.77	Malmborg, 1984 [25]
100 mg SD[a]	NA	NA	NA	0 – inf	37.4[#]	30.8[#]	0.82	Malmborg, 1984 [25]
200 mg SD[a]	2.61[#]	3.26[#]	1.25	0 – inf	40.9[#]	62.3[#]	1.52	Wojcicki et al., 1985 [26]
200 mg q24h[b,g]	3.17[#]	2.89[#]	0.912	0 – 24	32.0[#]	42.1[#]	1.32	Newton et al., 2005 [27]
200 mg q24h[b,g]	4.44[#]	4.05[#]	0.912	144 – 168	48.6[#]	58.6[#]	1.21	Newton et al., 2005 [27]
100 mg q24h[a,i]	3.26[#]	2.26[#]	0.70	312 – 408	37.3[#]	36.3[#]	0.97	Binh et al., 2009 [28]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**83%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
Lumefantrine								
480 mg SD[a,c]	7.91[#]	4.87[#]	0.62	0 – inf	207[#]	136[#]	0.66	Lefevre et al., 2002 [5]
480 mg SD[a,h]	8.92[#]	5.27[#]	0.59	0 – 264	236[#]	123[#]	0.52	Lefevre et al., 2013 [6]
480 mg BID (Day 3) PM[a,c]	10[#]	10.1[#]	1.01	62 – 480	383[#]	452[#]	1.18	Lefevre et al., 2002 [7]
480 mg BID (Day 3) PM[a,c]	11.6[#]	9.53[#]	0.82	60 – 324	418[#]	396[#]	0.95	Huang et al., 2012 [8]
	Within 1.5-fold		**50%**		**Within 1.5-fold**		**50%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Mefloquine								
250 mg SD[a,c]	0.31[#]	0.32[#]	1.02	0 – inf	116[#]	108[#]	0.93	Schwartz et al., 1982 [29]
1000 mg SD[a,c]	0.96[#]	1.27[#]	1.32	0 – inf	516[#]	430[#]	0.83	Schwartz et al., 1982 [29]
750 mg SD[a,g]	1.18[#]	1.18[#]	1.00	NA	NA	NA	NA	Boudreau et al., 1990 [30]
1500 mg SD[a,g]	1.44[#]	2.37[#]	1.64	NA	NA	NA	NA	Boudreau et al., 1990 [30]
750 mg SD[a,g]	1225	1169	0.95	0 – inf	393500	382473	0.97	Na-Bangchang et al., 1999 [31]
500 mg LD, 250 mg weekly (Day 140)[a,h]	1.42[#]	0.92[#]	0.65	3360 – 3528	174.9[#]	114[#]	0.65	Schwartz et al., 1987 [32]
	Within 1.5-fold		**66%**		**Within 1.5-fold**		**75%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Piperaquine								
1280 mg SD[n]	0.19[+]	0.24[+]	1.25	0 – 72	3.01[+]	3.46[+]	1.15	EMA Website, [33]
960 mg QD[o] (fasted, Day 3)	0.505[+]	0.37[+]	0.73	0 – 72	5.38[+]	3.62[+]	0.67	Eurartesim S06, Females <75 kg
960 mg QD[o] (fed, Day 3)	1.27[+]	0.97[+]	0.77	0 – 72	12.5[+]	10.6[+]	0.85	Eurartesim S06, Females <75 kg
960 mg QD[o] (fasted, Day 3)	0.28[+]	0.34[+]	1.11	0 – 72	3.93[+]	3.76[+]	0.96	Eurartesim S06, Males <75 kg
960 mg QD[o] (fed, Day 3)	1.12[+]	0.90[+]	0.80	0 – 72	10.7[+]	10.9[+]	1.02	Eurartesim S06, Males <75 kg
1280 mg QD[n] (fasted)	0.28[+]	0.32[+]	1.15	0 – 72	3.93[+]	3.46[+]	0.88	Eurartesim S06, Males ≥75 kg
1280 mg QD[n] (fed)	1.12[+]	1.05[+]	0.94	0 – 72	10.7[+]	12.9[+]	1.20	Eurartesim S06, Males ≥75 kg EMA Website, [33]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
Primaquine								
15 mg SD[a]	53	42	0.79	0 – inf	500	420	0.84	Mihaly et al., 1985 [12]
45 mg SD[a]	176	126	0.72	0 – inf	1700	1300	0.76	Mihaly et al., 1985 [12]
30 mg SD[g]	128	110	0.86	0 – inf	1130	1123	0.99	Hanboonkunupakarn et al., 2014 [13]
15 mg SD	65	53	0.82	0 – inf	468	509	1.09	Ward et al., 1985 [14]
15 mg QD (Day 14)	66	55	0.83	0 – inf	443	525	1.19	Ward et al., 1985 [14]
30 mg SD[f]	139	107	0.77	0 – inf	1180	1050	0.89	Jittamala et al., 2015 [15]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Proguanil								
200 mg SD[f,p]	170	176	1.04	0 – inf	2975	2878	0.97	Wattanagoon et al., 1987 [17]
200 mg SD EM[a,p]	NA	NA	NA	0 – inf	3396	1938	0.57	Helsby et al., 1990 [18]
200 mg SD PM[a,p]	NA	NA	NA	0 – inf	6563	3781	0.58	Helsby et al., 1990 [18]
200 mg SD EM[a,p]	209	149	0.71	NA	NA	NA	NA	Helsby et al., 1993 [19]
200 mg QD (Day 14) EM[a,p]	190	188	0.99	NA	NA	NA	NA	Helsby et al., 1993 [19]
200 mg SD PM[a]	273	187	0.68	NA	NA	NA	NA	Helsby et al., 1993 [19]
200 mg QD (Day 14) PM[a]	338	270	0.80	NA	NA	NA	NA	Helsby et al., 1993 [19]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**33%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Pyrimethamine								
100 mg SD[a]	771	594	0.77	0 – 336	76.2	67.8	0.89	Cavallito et al., 1978 [34]
25 mg SD[a,l]	214	145	0.68	0 – 264	19.1	17.5	0.91	Weidekamm et al., 1982 [35]
25 mg SD[a,l]	130	144	1.11	0 – inf	18.6	22.0	1.18	Edstein, 1987 [36]
25 mg (once weekly, 8th week)[a,m]	116	107	0.92	0 – inf	10.7	10.6	0.99	Edstein et al., 1990 [37]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
Pyronaridine								
6 mg/kg pyronaridine salt SD[a,j]	0.186	0.212	1.14	0 – inf	8.71	11.0	1.27	Wattanavijitkul, 2010 [38]
9 mg/kg pyronaridine salt SD[a,j]	0.262	0.318	1.21	0 – inf	7.67	16.5	2.15	Wattanavijitkul, 2010 [38]
12 mg/kg pyronaridine salt SD[a,j]	0.467	0.424	0.91	0 – inf	12.4	22.0	1.78	Wattanavijitkul, 2010 [38]
15 mg/kg pyronaridine salt SD[a,j]	0.792	0.530	0.67	0 – inf	20.8	27.6	1.33	Wattanavijitkul, 2010 [38]
410 free base, 3 daily doses[a,c]	0.370	0.489	1.32	48 – 960	25.9	40.6	1.57	Morris et al., 2014 [39]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**40%**	
	Within 2-fold		**100%**		**Within 2-fold**		**80%**	
Quinine								
600 mg SD	3100	3060	0.99	0 – inf	52000	44800	0.86	Ho et al., 1999 [40]
550 mg SD	2848	2884	1.01	0 – inf	50890	38390	0.75	Mirghani et al., 1999 [41]
600 mg SD	4600	3023	0.66	0 – inf	66000	44386	0.67	Wanwimolruk et al., 1995 [42]
	Within 1.5-fold		**67%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Sulfadoxine								
500 mg SD[c]	63.2[#]	46.17[#]	0.73	0 – inf	14168[#]	10733[#]	0.76	Weidekamm et al., 1982 [35]
1500 mg SD[c]	142[#]	154[#]	1.09	0 – inf	33284[#]	32599[#]	0.98	Karunajeewa et al., 2009 [43]
500 mg weekly (20 weeks)[c]	121[#]	96.3[#]	0.79	3360 – 3528	12465[#]	11321[#]	0.91	Schwartz et al., 1987 [32]
500 mg SD[d]	77.0[#]	66.1[#]	0.86	0 – inf	26689[#]	14195[#]	0.53	Sarikabhuti et al., 1988 [44]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**75%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
Tafenoquine								
300 mg SD	186	273	1.47	0 – 72	10611	15056	1.42	Green et al., 2014 [45]
600 mg SD	422	389	0.92	0 – 72	22986	23374	1.02	Green et al., 2014 [45]
400 mg QD (3 days)	724	686	0.95	0 – 72	41896	43990	1.05	Green et al., 2014 [45]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

Compound (regimen)	C_{max} (ng/mL)			AUC window (h)	AUC (ng/mL·h)			Reference
	Obs	Sim	Sim/Obs		Obs	Sim	Sim/Obs	
DSM265								
400 mg SD[a]	11500	8309	0.72	0 – inf	1210000	1052927	0.87	McCarthy et al., 2017 [46]
600 mg SD[a]	15500	12464	0.80	0 – inf	2140000	1579395	0.74	McCarthy et al., 2017 [46]
800 mg SD[a]	19100	16619	0.87	0 – inf	2220000	2105845	0.95	McCarthy et al., 2017 [46]
1200 mg SD[a]	34800	24928	0.72	0 – inf	4720000	3158787	0.67	McCarthy et al., 2017 [46]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
DSM450								
400 mg SD[a]	1070	873	0.82	0 – inf	271000	337751	1.25	McCarthy et al., 2017 [46]
600 mg SD[a]	1380	1309	0.95	0 – inf	477000	506626	1.06	McCarthy et al., 2017 [46]
800 mg SD[a]	1920	1746	0.91	0 – inf	454000	675501	1.49	McCarthy et al., 2017 [46]
1200 mg SD[a]	3070	2619	0.85	0 – inf	1170000	1013252	0.87	McCarthy et al., 2017 [46]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**100%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	
MMV048								
40 mg SD[a]	272.7	253	0.93	0 – inf	30320	55258	1.82	McCarthy et al., 2020 [47]
80 mg SD[a]	561.0	506	0.90	0 – inf	82680	110516	1.34	McCarthy et al., 2020 [47]
120 mg SD[a]	1094.0	759	0.69	0 – inf	137800	165774	1.20	McCarthy et al., 2020 [47]
	Within 1.5-fold		**100%**		**Within 1.5-fold**		**67%**	
	Within 2-fold		**100%**		**Within 2-fold**		**100%**	

[a]healthy volunteers; [b]malaria-infected individuals; [c]Caucasian; [d]South-East Asian; [e]African; [f]Chinese, [g]Thai, [h]Brazillian, [i]Vietnamese, [j]Korean, [k]Indian,

[l]Co-administered with 500 mg sulfadoxine, [m]Co-administered with 100 mg dapsone, [n]tetraphosphate salt, simulated free base dose = 739 mg, [o]tetraphosphate salt, simulated free base dose = 554 mg, [p]dose corrected to free base for simulations.

[#]µg/mL for C_{max} or µg·h/mL AUC; [+]mg/L for C_{max} or mg·h/L for AUC; [*]µM for C_{max} or µM·h AUC

SD, single dose; QD, once a day; BID, twice a day; EM, extensive metabolisers; PM, poor metabolisers; Sim, simulated; Obs, observed; Sim/Obs, the ratio of simulated to clinically observed PK parameters; inf, infinity

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